SANS Data Analysis Tutorial

11/2000 version

This tutorial guides you through the steps of modeling your averaged (1-D) SANS data using available model functions and IGOR Pro's built in non-linear least squares fitting routines. Detailed statistical information about the goodness-of-fit are provided, including chi-squared error, uncertainty in fitted parameters, confidence intervals, and covariance. This demo only uses the basics of IGOR's curve fittng capabilities. Refer to IGOR Pro's online Curve Fitting help for the full details.

NOTE: You DO NOT need to purchase IGOR Pro to model your data. You can use either the (free) Demo version of IGOR Pro, or the full version. IGOR Pro 3.1x or higher is required. The descriptions of each step are taken using IGOR Pro v4.0. The appearance of the dialogs will be somewhat different if using IGOR Pro 3.1x. (*The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.)

IGOR Pro is available at: <http://www.WaveMetrics.com> (v. 4.0 is the current version).

Overview of Fitting

The general procedure for fitting a model to your data is:
1) Load in your SANS data
2) Plot a model function
3) Visually adjust the model parameters
4) Set up the curve fitting parameters
5) Do the fit
6) Make publication-quality graph

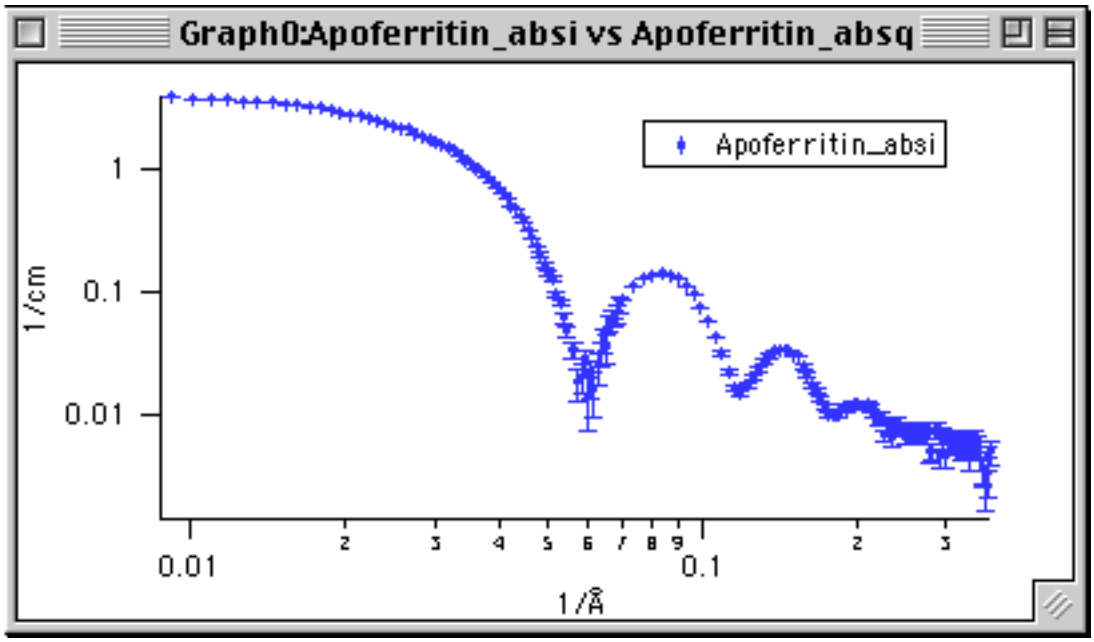
Open the experiment file "Model_Fit_Demo.pxt" containing the fitting function. A separate file of sample data file is also included. This data "Apoferritin.abs" is the output data file from the SANS Data Reduction tutorial.

The demo experiment includes only a single model function. Instructions for downloading and installing additional model functions are available at:
<http://www.ncnr.nist.gov/programs/sans/igor2.html>

Loading SANS Data

If you haven't done so, open the experiment file "Model_Fit_Demo.pxt". There will now be three menu items under the Macros menu. Select "LoadOneDData"

and you will be prompted to select a data file. Choose the Apoferritin.abs file, and it will automatically be loaded and graphed.



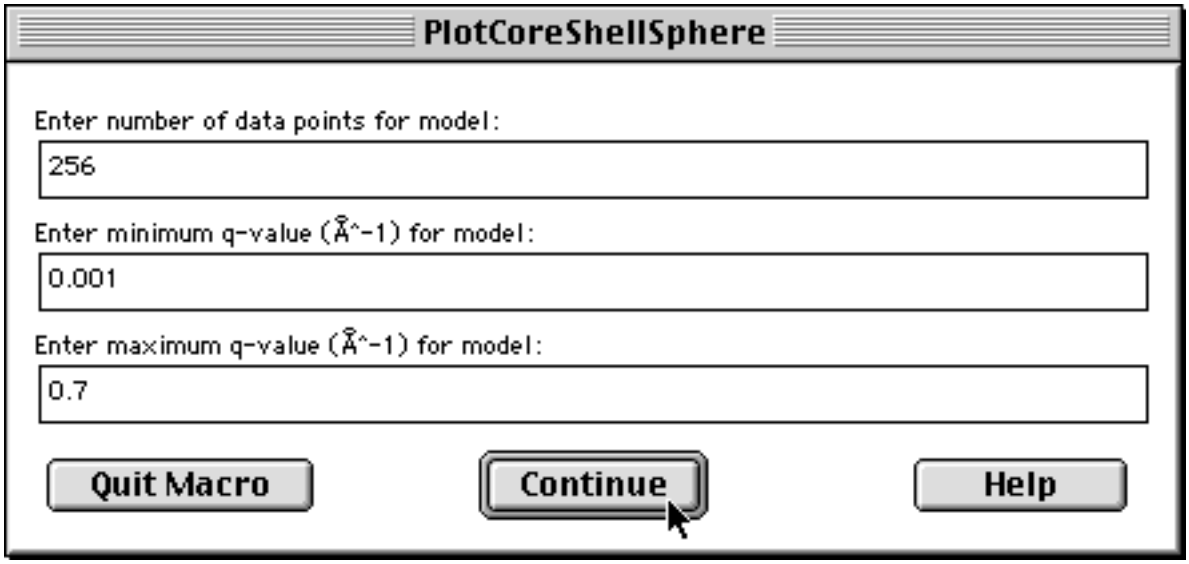
The Apoferritin.abs data file contains six columns of data. The macro automatically names and tags each of these columns to uniquely identify them. Select the Data Browser from the Data menu, and you will see seven "waves" listed:

Apoferritin_absq	"q" = q-values
Apoferritin_absi	"i" = intensity
Apoferritin_abss	"s" = standard deviation of intensity
Apoferritin_absqb	"qb" = mean q-value (for resolution)
Apoferritin_abssq	"sq" = resolution standard deviation (resolution)
Apoferritin_absfs	"fs" = beamstop shadowing (resolution)
Apoferritin_abswt	"wt" = weighting (=1/std dev of intensity)

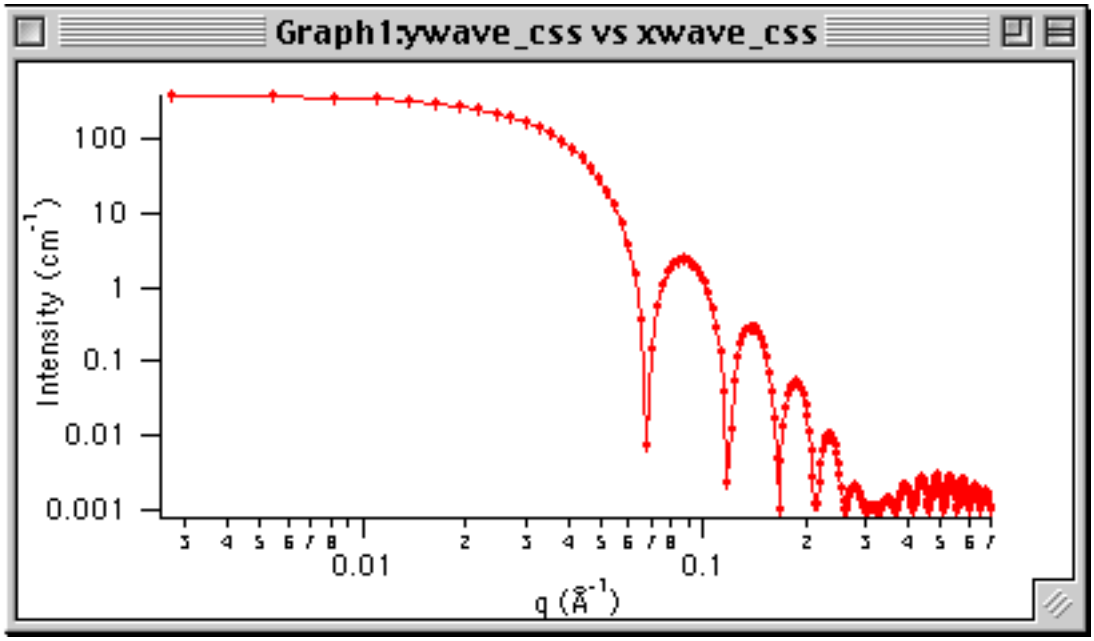
Plotting a Model Function

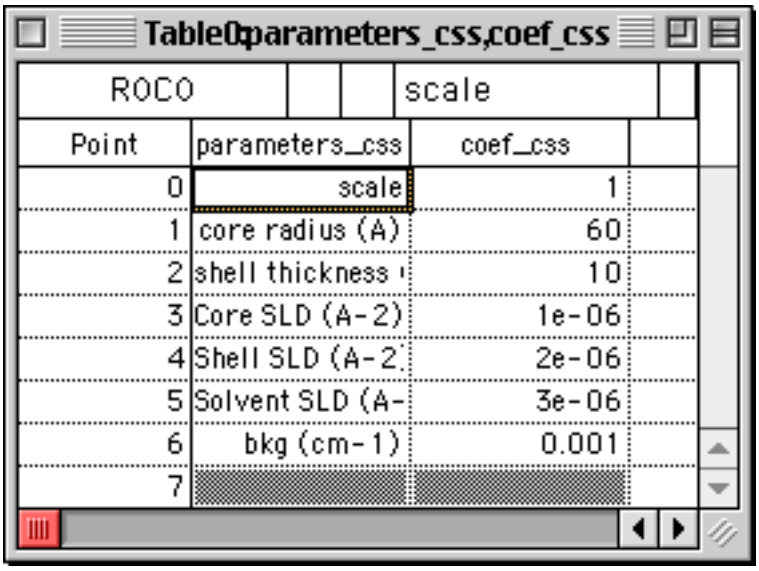
Model functions are plotted by selecting the appropriate "Plot..." Macro. This macro will create the x and y waves of data, a table of adjustable parameters, and graph the model

function. Choose "PlotCoreShellSphere" from the Macros menu:



click "continue" to accept the default ranges, and the following graph and table are generated.

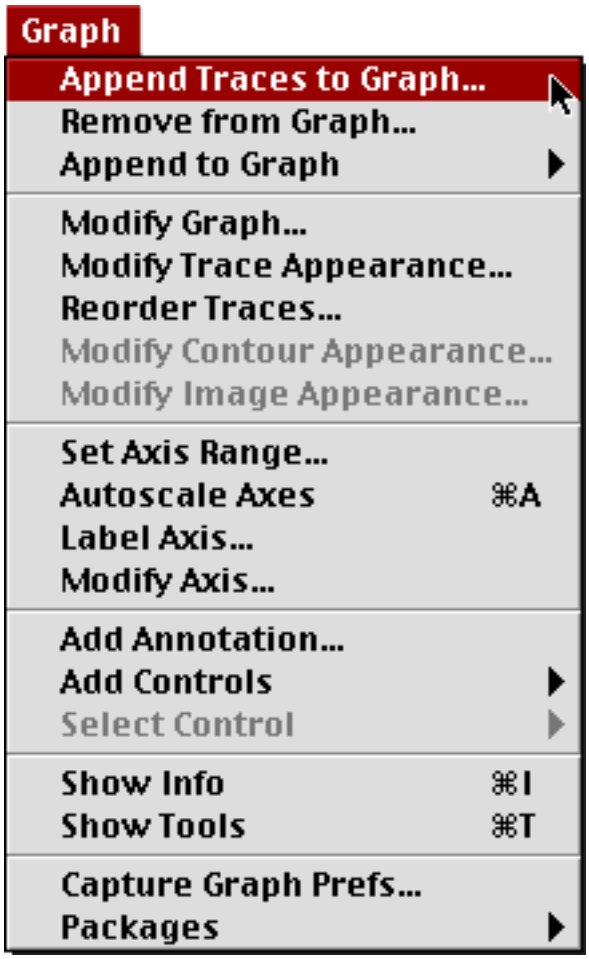




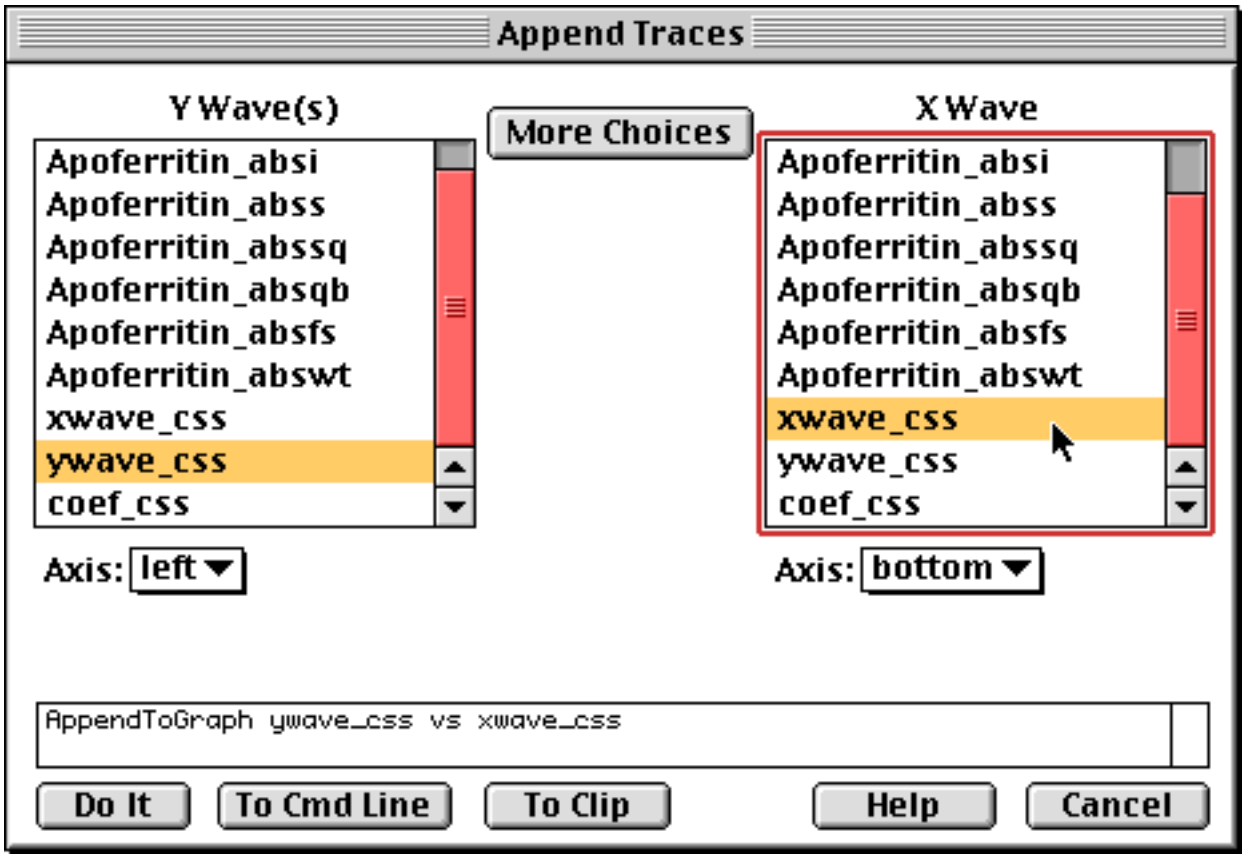
Drag the graph to the side to reveal the table of fitting coefficients, and resize the windows as you choose. The model function macros create x and y values with appropriate extensions, xwave_**ext** and ywave_**ext.** Coefficient and parameter waves are likewise created for the table. For the Core-shell sphere model, the extension is "css". If you're curious about the details of the model calculation, documentation of each model is available and the code is visible under the Windows->Other Windows menu.

Testing the Model

What we really want to see is how the model compares to the experimental data. Add the model data to the experimental data by bringing the graph of the experimental data to the front, then choosing "Append Traces to Graph..." from the Graph menu. Note that the Graph menu is visible only if there is a graph window on top.



From the dialog presented, choose "ywave_css" and "xwave_css" and the y and x-axes respectively, and "Do It":



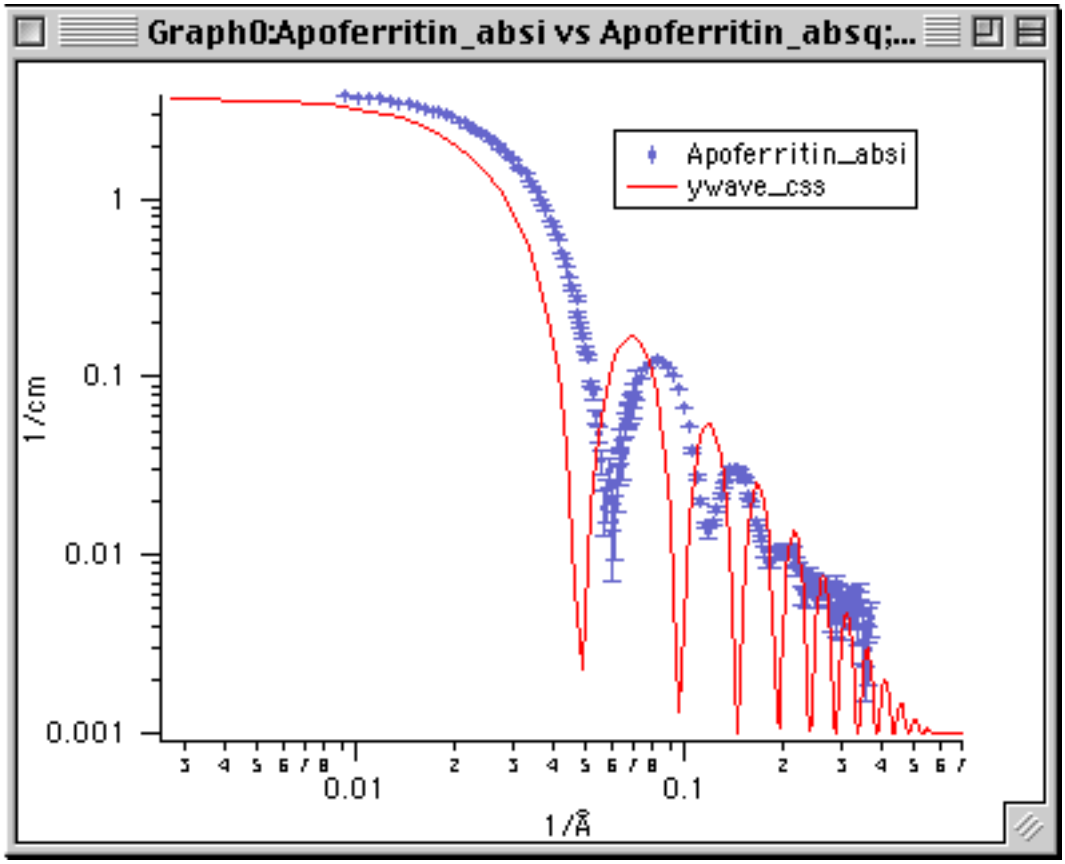
The model data has been appended to the graph, and is a poor representation of our experimental data. Let's see how changing the parameters affects the model. The model intensity "ywave_css" is a "dependent object" - that is, the wave depends on the parameter values in the table - change any of the values, and the data in the graph is automatically updated. For the apoferritin sample, we know that it was prepared in deuterated water at a concentration of 1% by volume. From the crystal structure of the protein, it is also known that the structure resembles a hollow spherical shell of protein. So set the scale equal to the volume fraction, and the scattering length densities of the solvent and the core (which is filled with solvent) to the scattering length density of D_2O. If you don't know this number, a very useful tool for calculating scattering length densites can be found at: <http://www.ncnr.nist.gov/resources/>, along with a growing list of tools for planning your experiment at NIST.

The table should look like this:

Table0:parameters_css,coef_css

ROC1		0.01
Point	parameters_css	coef_css
0	scale	0.01
1	core radius (A)	60
2	shell thickness (A)	10
3	Core SLD (A-2)	6.35e-06
4	Shell SLD (A-2)	2e-06
5	Solvent SLD (A-2)	6.35e-06
6	bkg (cm-1)	0.001
7		

and the graph, now much closer to the data:

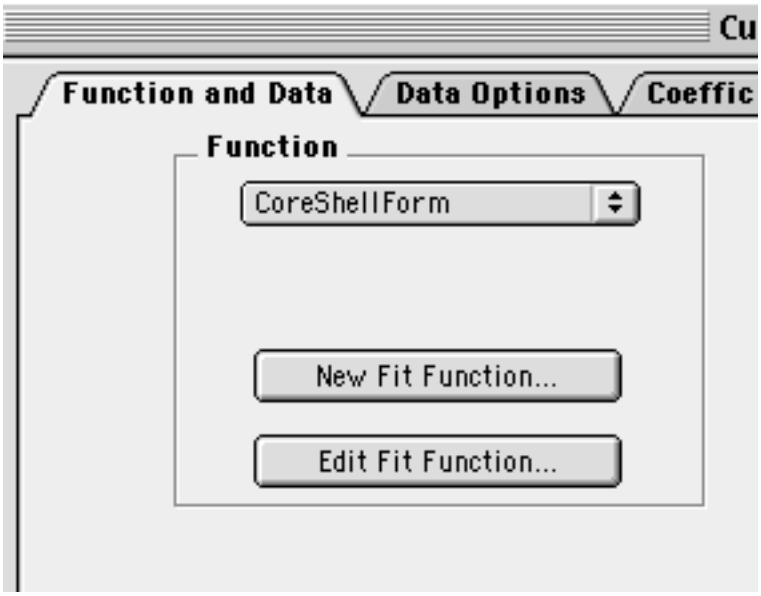


You can play with the parameters more, if you like. These values should be close enough to use as initial guesses for the non-linear fitting. Depending on the particulars of the model, the initial guess can be very poor, or may need to be relatively close.

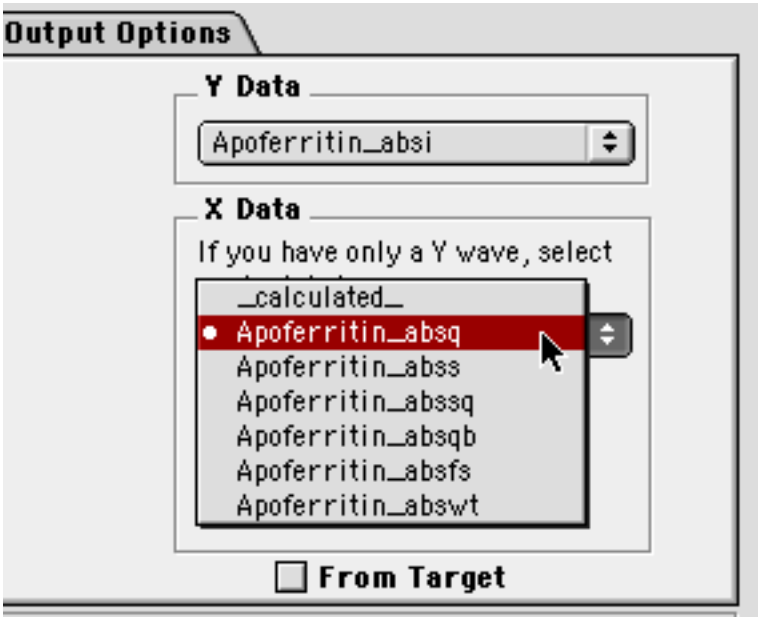
Setting up the Fit Parameters

You're ready to fit the core-shell model to the data now. Select "Curve Fitting" from the Analysis menu

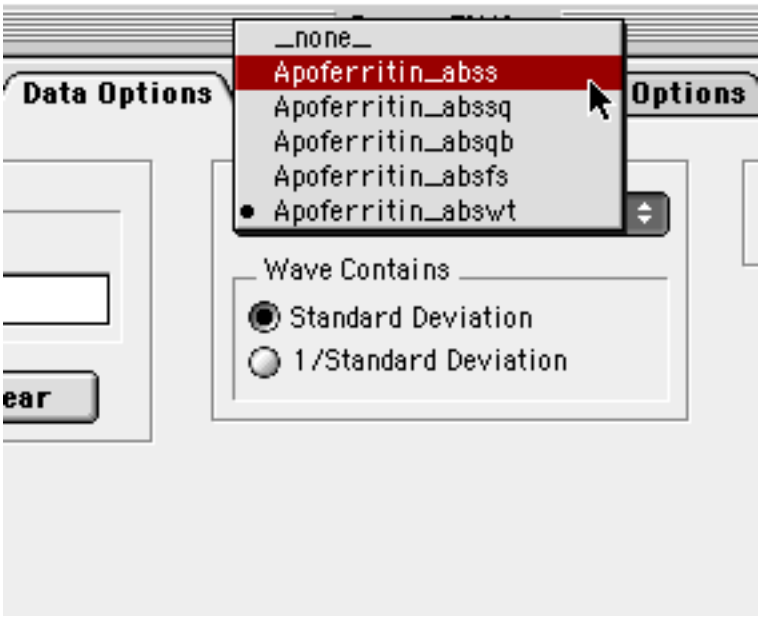
To get the following multi-tabbed dialog (IGOR Pro 3.xx does not have these tabs). Under the Function and Data" tab, select the model function "CoreShellForm" from the list (You may need to select "Show Old-Style Functions" to see the scattering models).



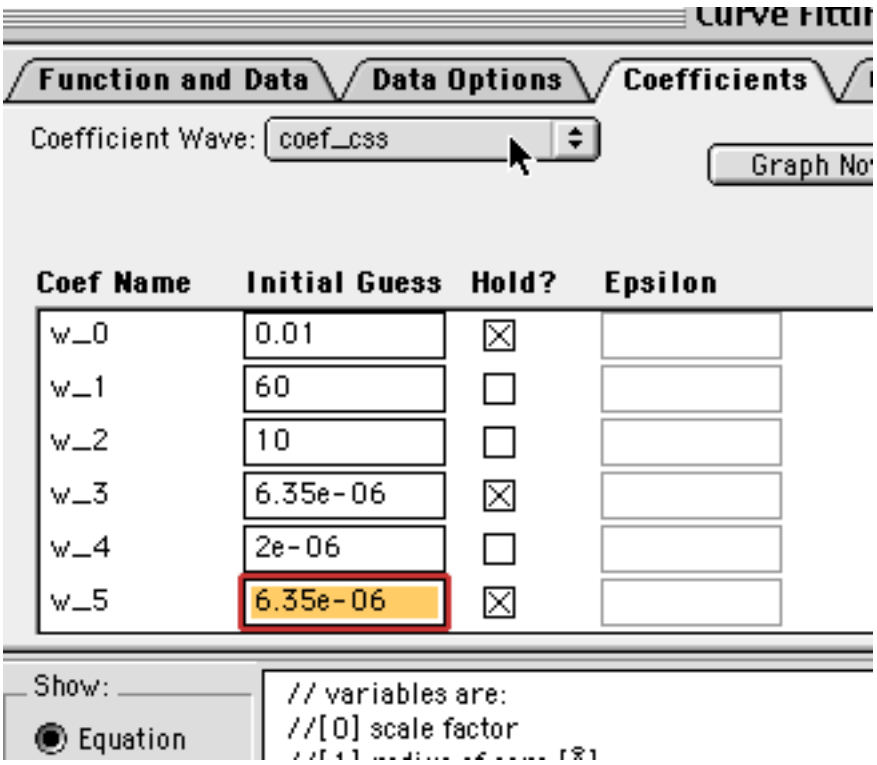
Then select your y and x data. The y data is the intensity, "Apoferritin_absi", and the x data is q-values, "Apoferritin_absq".



From the "Data Options" tab, select the standard deviation of the intensity, "Apoferritin_abss" as the weighting, and mark that it contains the standard deviation, not the recoprocal. The "Apoferritin_abswt" wave contains the reciprocal of the standard deviation, and is the correct weighting wave to use with IGOR Pro 3.xx.



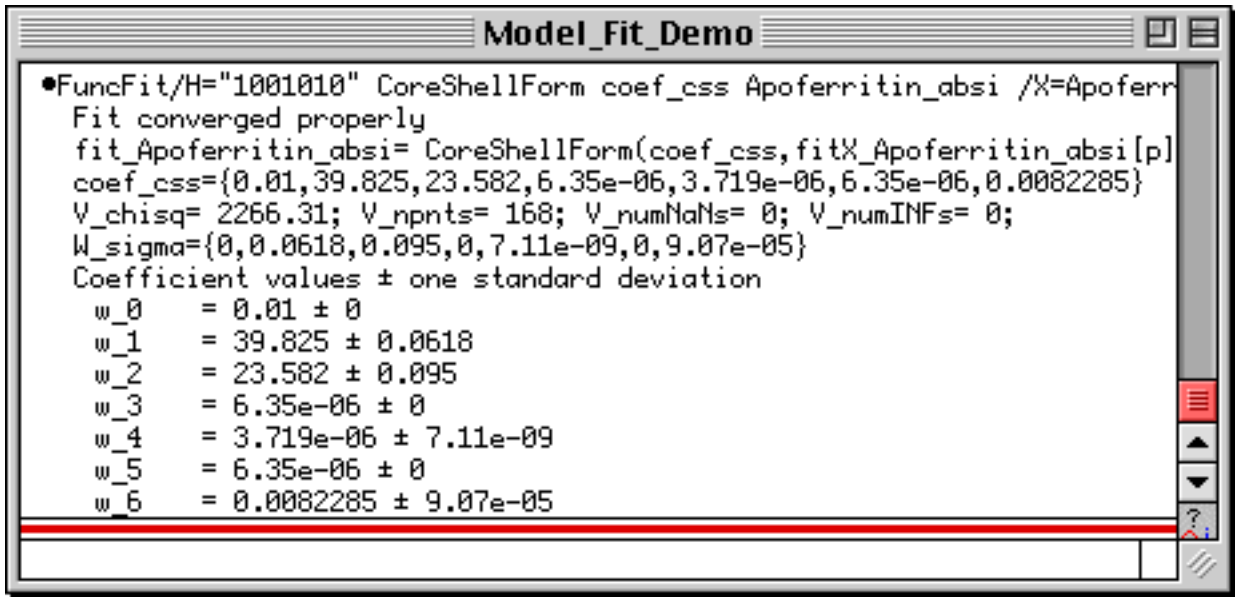
From the "Coefficients" tab, select the coefficient wave "coef_css", which has our "good" guesses. The current values appear (you could further adjust the initial guesses here, too). Since we know the values of the scale and two of the scattering length densities, we want to hold these values fixed during the fitting. Select "hold" for these parameters - refer back to the parameter table if you need to.

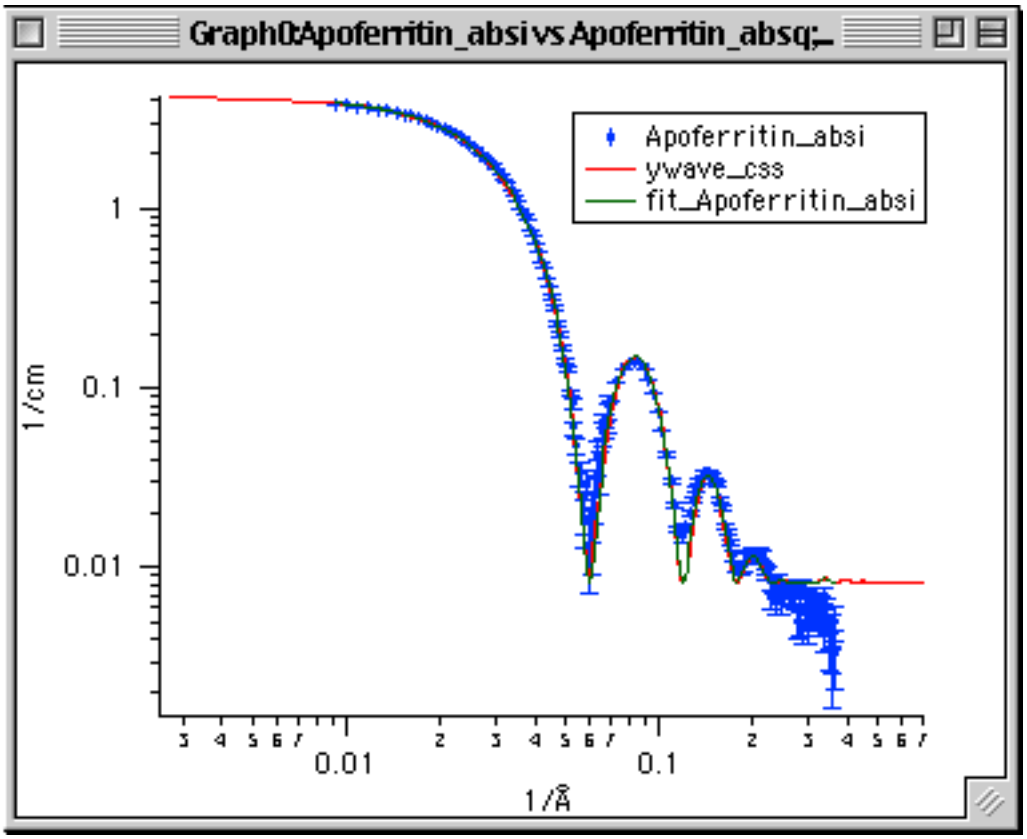


From the "Output Options" tab, leave the default values.

Fit Results

Click "Do It", and the fit will be performed, updating the model as it (quickly) converges to a solution. Click "OK" to accept the results of the fit. The best-fit parameters and one standard deviation are reported to the command window at the bottom of the screen:





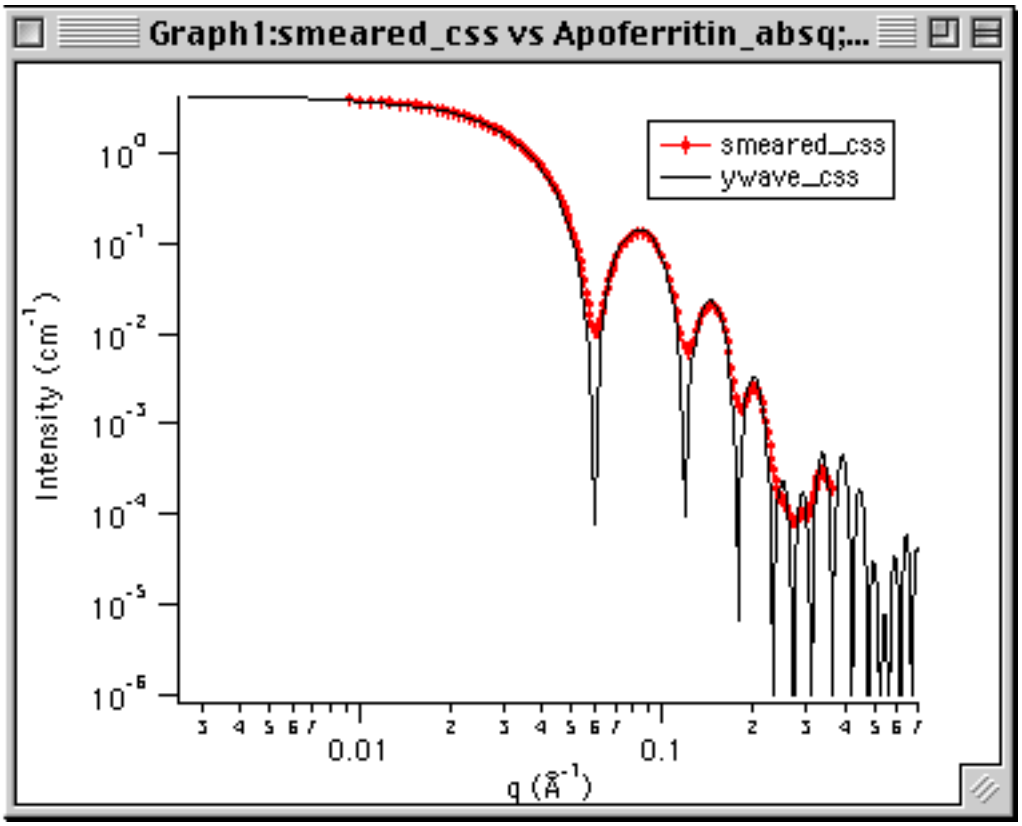
The fit is not too bad, but could be better. The CoreShellForm model did not take the instrumental resolution function into account, and for this example, is likely the cause of the artificially high background value at high q ($q > 0.2$ Å^{-1}).

Plotting a Resolution Smeared Function

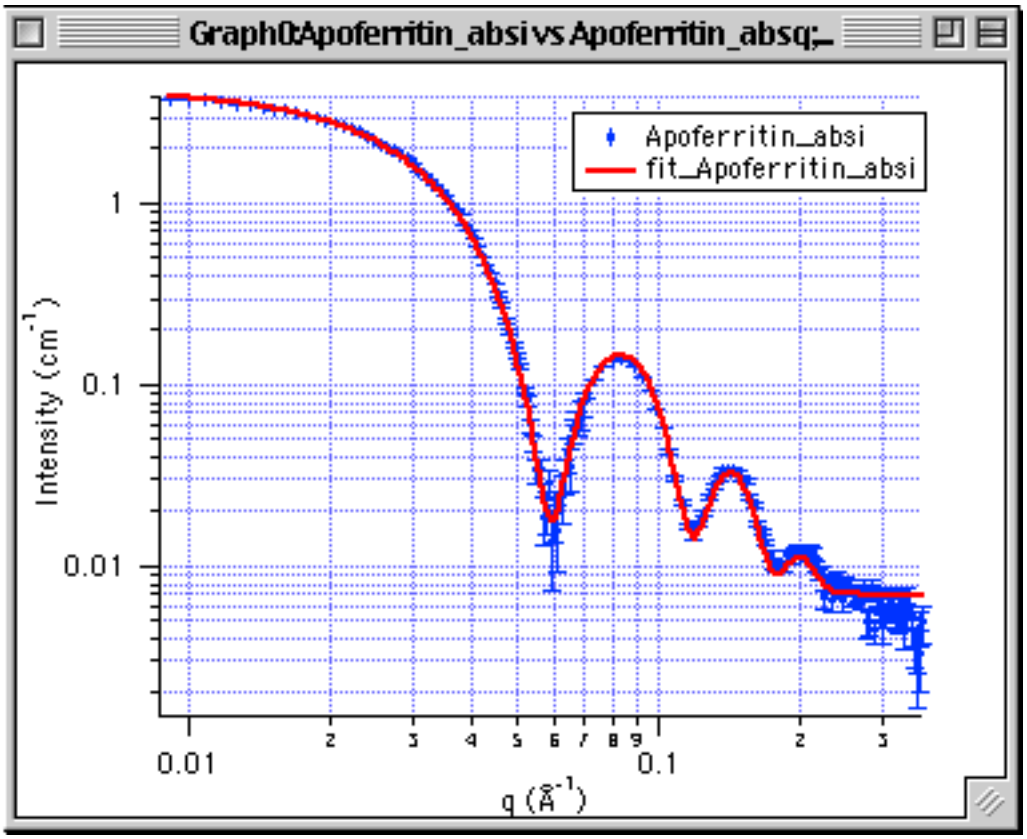
Including instrumental resolution effects into the model caluculation is easy, and in some cases can have a significant effect on the best-fit parameters. The extra three columns of data in the apoferritin data file (and in all SANS data files) is the resolution information that describes the "smearing" effect of the wavelength distribution, apertures, detector resolution, etc... The model function is smeared with the resolution information, and then the smeared model is fitted to the (smeared) experimental data.

NOTE: The resolution information that is used for the smearing calculation is taken from the most recent 6-column data file that was read into the experiment. You should load the experimental data of interest and finish with the smeared modeling of that dataset before loading another.

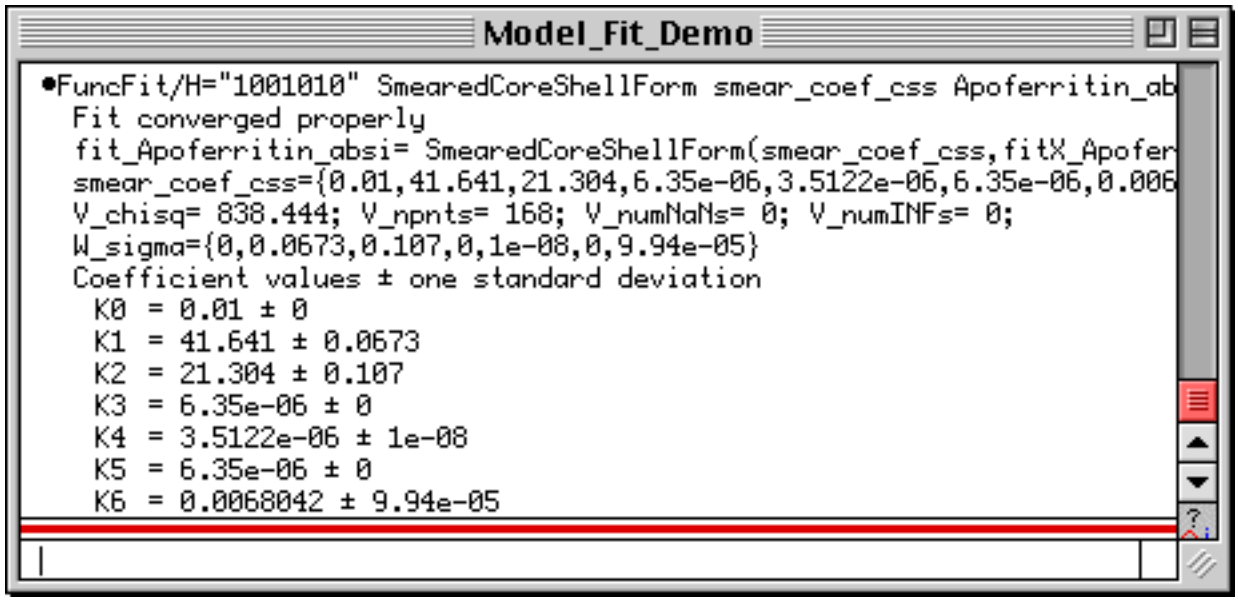
Select "PlotSmearedCoreShellSphere" from the macros menu. No dialog to select the number of data points or the q-range is presented, since these values are set by the experimental data. Append the unsmeared data to the smeared data, change the smeared coefficients to the best-fit values from the unsmeared model, and set the background value of each coefficient table to zero. You should have a plot something like this, where the oscillations of the model have been smeared out by the resolution function.



Fitting the smeared model to the data follows the same sequence as for the unsmeared model. Bring the graph of experimental data to the front and select "Curve Fitting..." from the Analysis menu. This time, select the "SmearedCoreShellForm" function, and the "smear_coef_css" coefficients. All other choices should be the same as for the previous fit. Once all is set, click "Do It", and the fit is done. The fit should be rather quick this time, since the initial guesses are very good. The final fit is visually "better" when resolution is included.



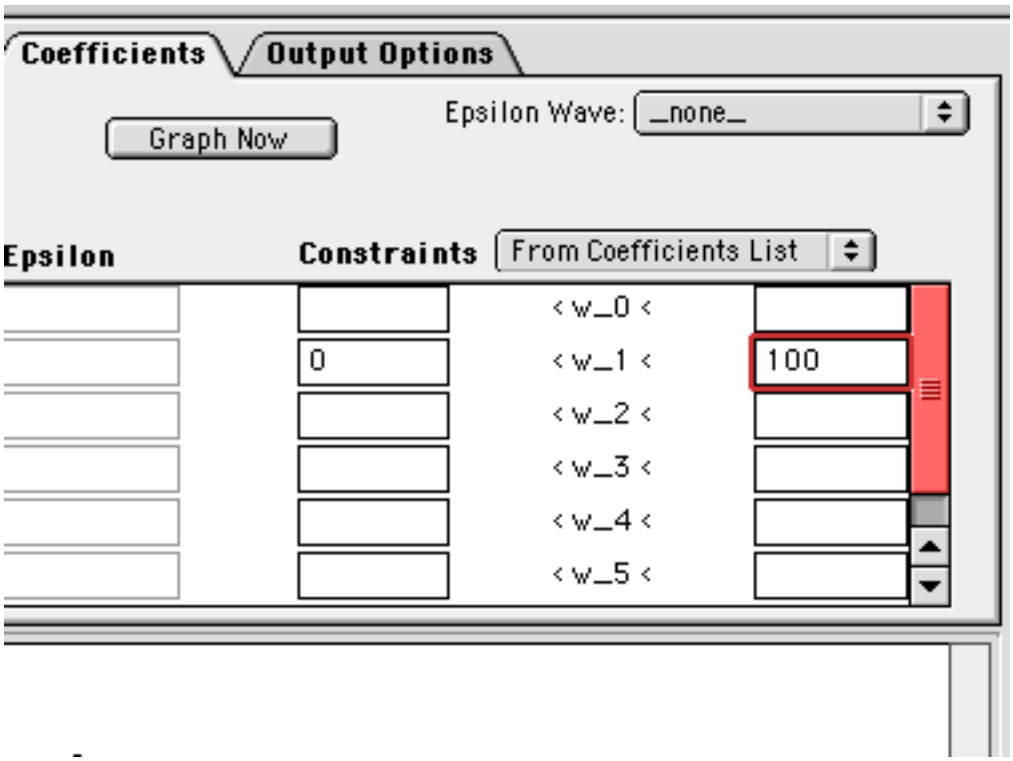
The best-fit coefficients from this fit are also reported in the command window, and can be compared to the results of the unsmeared fit.



Parameter Constraints

Although not necessary in this simple example, constraints can be placed on coefficient values during the fitting. Bounded coefficients are often critical for highly nonlinear functions, or helpful in cases where a range of allowable values can be set. Constraints are set in the Curve

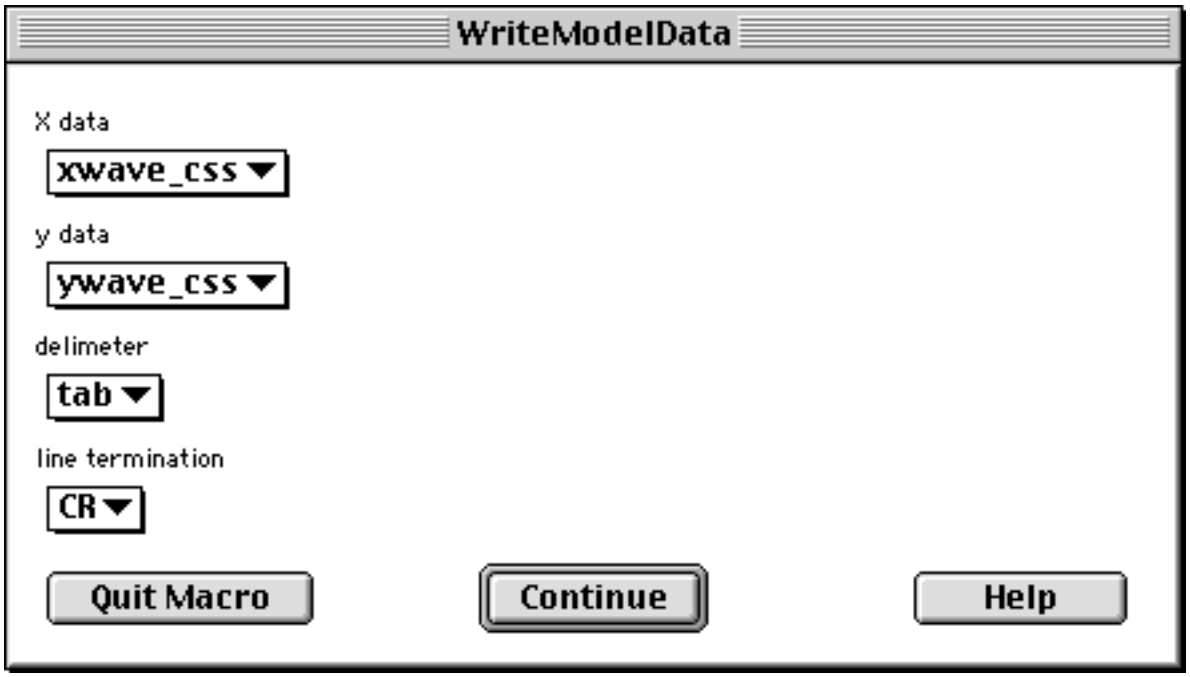
Fitting dialog, under the "Coefficients" tab:



Simple bounds can be set here, or more complex relations between the variables can be created. See the IGOR Pro help file Fitting With Constraints for all the details.

Exporting SANS Models

You can export the model calculations as x-y data, in a two-column ASCII format. Choose "WriteModelData" from the Macros menu, and the following dialog appears:



Choose the desired waves from the popup menus, select the delimeter (either a tab or 3 spaces) and the line terminator. Macintosh uses a carriage return (CR), Unix uses linefeed (LF) and Windows uses both (CRLF). Continue, and you will be prompted for a filename for the exported data. If you have a full version of IGOR Pro, you have a variety of other save options available using "Save Waves..." under the data menu.